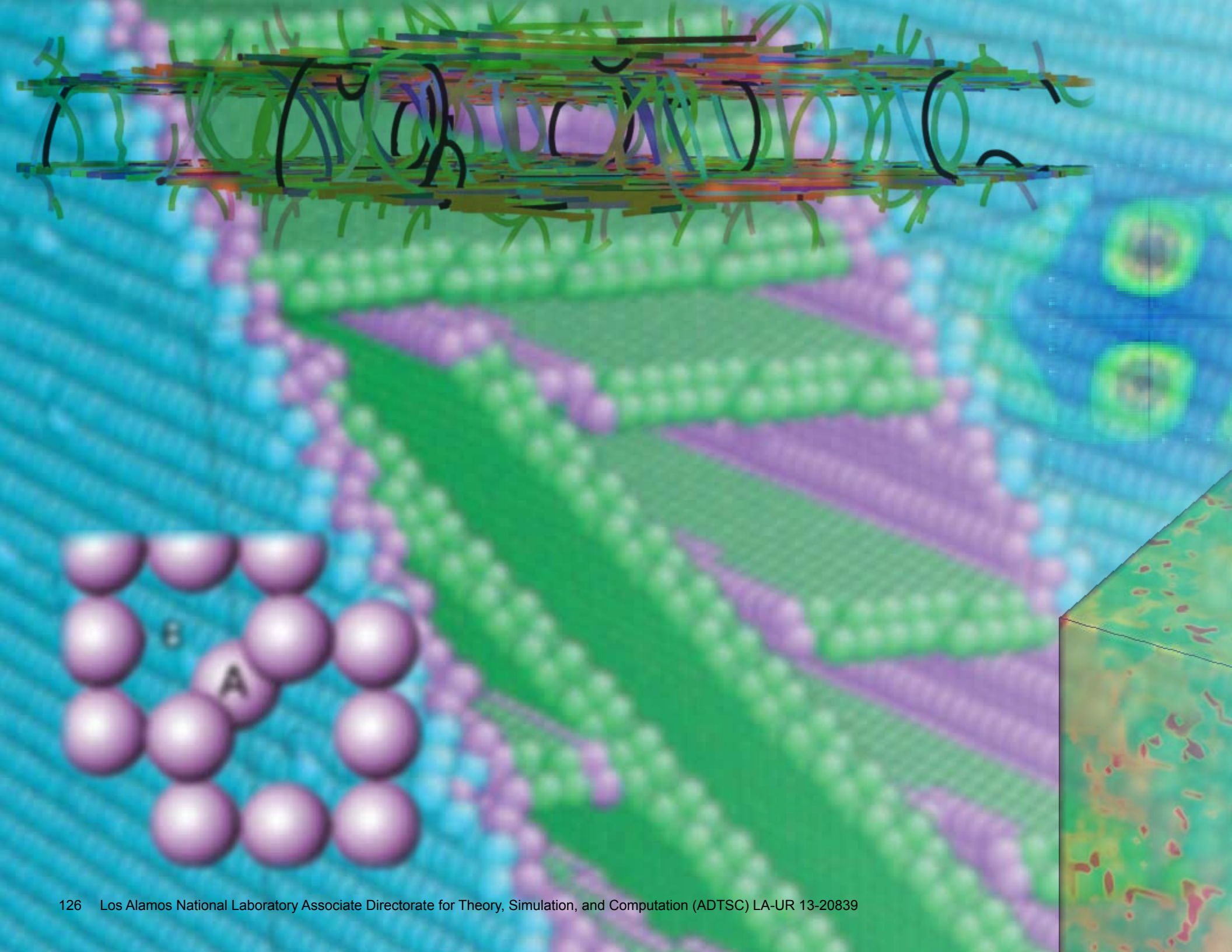
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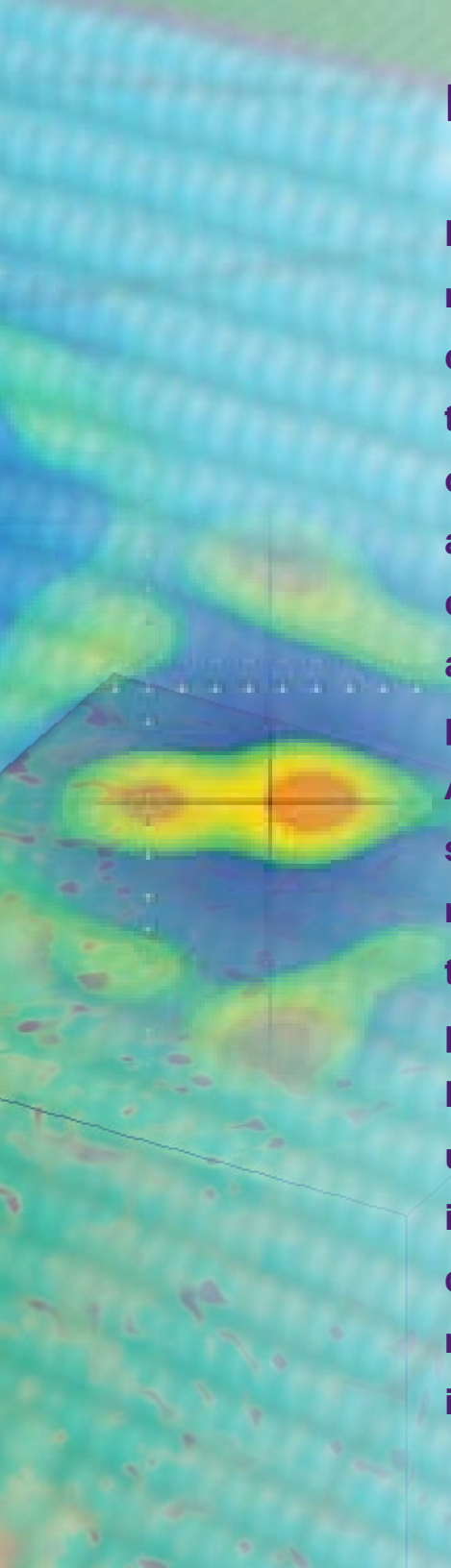

# Materials Science

Researchers at LANL conduct fundamental research into the state and nature of materials, provide new theories for materials behavior, and create and provide new constitutive properties models and parameters for a wide variety of simulation tools in use or under development around the world. Not surprisingly, much of our work deals with materials in extreme conditions—highly stressed, shocked, and high-radiation field environments. This work with materials in extreme conditions in particular supports the LANL grand vision to design and construct a world-class facility called MaRIE (Matter-Radiation Interactions in Extremes) to predict and control material performance under dynamic and harsh conditions. Articles in this section explore methods to increase the performance of electronic structure and quantum-based molecular dynamics simulations, coupling a thermal mechanical model with a thermal ignition model for energetic materials, predicting the evolution of crystallographic texture for rolled metals, discovering the design principles for large spin and phonon fluctuations, calculating transition rates in large-scale materials, modeling dislocation processes of nanolayered composites under shock compression, capturing the fundamental physics of dislocation-interface interactions, and simulating dynamics and pattern formation of driven dislocation assemblies. This broad range of physical modeling approaches, mathematical and numerical algorithms, and multiple length and time scales is illustrative of the breadth and depth of our capabilities in this arena.